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A SIMULATION MODEL FOR MATERIAL ACCOUNTING SYSTEMS*

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Abstract

A general-purpose model that was developed to simulate the operation of a chemical processing facility for nuclear materials has been extended to describe material measurement and accounting procedures as well. The model now provides descriptors for material balance areas, a large class of measurement instrument types and their associated measurement errors for various classes of materials, the measurement instruments themselves with their individual calibration schedules, and material balance closures. Delayed receipt of measurement results (as for off-line analytical chemistry assay), with interim use of a provisional measurement value, can be accurately represented. The simulation model can be used to estimate inventory difference variances for processing areas that do not operate at steady state, to evaluate the timeliness of measurement information, to determine process impacts of measurement requirements, and to evaluate the effectiveness of diversion-detection algorithms. Such information is usually difficult to obtain by other means. Use of the measurement simulation model is illustrated by applying it to estimate inventory difference variances for two material balance area structures of a fictitious nuclear material processing line.

1. Introduction

The Safeguards Systems Group has been engaged for some time in the development of a computer simulation model for the Los Alamos Plutonium Facility, and we have previously reported on some of the features of this model.[1] The model has been designed to permit simulation of facility operation at almost any desired level of detail, from gross-scale representations where the "unit processes" are entire process lines and the time steps are measured in weeks or months to fine-scale descriptions in which every item of process equipment, every process step, and every operator procedure are accounted for in detail. In addition, though the simulation model was developed specifically to model the Plutonium Facility, we have constructed it so that the facility description used by the model is contained entirely in data files. As a consequence the simulation model is generic in character and can be applied to any nuclear material processing facility that has a process logic similar to that of the Plutonium Facility by simply constructing the appropriate data files. This generic character of the model is demonstrated in Ref. 1.

We have now extended the model to permit the simulation of material measurements, material balance closures, inventories, and other operations related to material accounting. In keeping with the spirit of the previous version of the model, we have structured the accounting and measurement additions to the model so that all facility-specific accounting and measurement information is also contained in data files. In the following sections we shall discuss the motivation for simulating material measurements, describe the measurement enhancements we have made to the model, and present the results of an example application of the extended simulation model.

2. Why Simulate Measurements?

All facilities possessing significant quantities of special nuclear materials (SNM) are required to maintain material measurement and accounting programs and to meet certain standards with respect to the accuracy and timeliness of material accounting information. The two methods most often used to estimate the accuracy of material accounting information are simulation and propagation of errors. On comparing these two methods one finds that there are a number of significant advantages to the use of a measurement simulation approach, particularly when--as in the case described here--the measurement simulation appears in the context of a detailed process simulation and all facility information is contained in data files. These advantages of the simulation approach include the following:

1. Simulation can be used to determine limits of error of inventory differences (LEIDs) for non-steady-state process operation.

2. Simulation can provide information on the timeliness of measurement results.

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3. Simulation gives information on the process impacts of measurement requirements, including operator time utilization and delays due to measurement instrumentation bottlenecks.

4. Correlation effects are automatically accounted for in simulations, and require no special consideration. In addition, arbitrary instrument calibration schedules can be used without difficulty.

5. Simulation allows one to use a variety of process holdup models with different holdup-model choices for different items of process equipment. Furthermore, process cleanouts can be scheduled at will. One can estimate the anticipated effects of holdup on inventory differences (IDs) after process cleanout or upon startup of a new facility.

6. The choices of measuring instruments, boundaries of material balance areas, etc., can be varied easily to aid in evaluating possible improvements to the material accounting system.

7. The measurement simulation can serve as a realistic test bed for decision-making algorithms for the detection of material diversion.

The simulation method also has disadvantages relative to the propagation-of-errors approach, including the following:

1. Simulation usually requires much more facility information than does the propagation-of-errors approach.

2. Determination of LEIDs by simulation requires a great deal more computer time than does the propagation-of-errors method.

For these reasons it is often appropriate to use the propagation-of-errors approach in preliminary design and scoping studies and to employ simulations of the kind described here for more detailed evaluation of final designs or of existing material accounting systems.

3. Accounting and Measurement Elements of the Simulation Model

The facility simulation model as previously constructed already contained a rather complete representation of material processing procedures, including unit process operations, material flows and transformations, and operator utilization. In order to also permit simulation of material measurements and other material accounting procedures, we have added descriptions of the following elements to the model.

Material balance areas. Any number of material balance areas (MBAs) may now be defined for the facility. Every vault area and in-process storage area must be assigned to an MBA. Each MBA has its own balance closure schedule, and the frequency of balance closures currently can be daily, weekly, biweekly, monthly, bimonthly, semiannually, annually, or biannually.

Measuring instrument types. Any number of measuring instrument types can be defined for the facility. Each measuring instrument type can have an arbitrary number of material accuracies specified for it. Each material accuracy describes the accuracy characteristics of the measuring instrument type for some subset of the SNM categories processed by the facility and has associated with it a precision uncertainty, a calibration uncertainty, a measurement time duration, and a delay period between the time the measurement is performed and the time the measurement result is available. The precision and calibration uncertainties each consist of two random distributions, one for the additive error and one for the multiplicative component of the error. The possibility of a delayed measurement result is provided to describe such measurement processes as "wet chemistry."

Measuring instruments. An arbitrary number of measuring instruments can be provided for the facility. Each measuring instrument must be of one of the types defined for the facility, and has its own individual calibration schedule. The calibration frequency can be any of the choices specified above for material balance closures. When a measuring instrument is calibrated at the beginning of program execution or at a subsequent scheduled calibration, the additive and multiplicative calibration distributions for the instrument type are used to generate a calibration error for every material accuracy class; and these calibration errors are retained until the next calibration. When the measuring instrument is used to perform a measurement, the additive and multiplicative precision distributions for the appropriate material accuracy class of the instrument type are used to produce a precision error, and this is combined with the current calibration error for the material accuracy class to yield the total error in the measured value.

SNM/bulk determination methods. One or more SNM/bulk determination methods can be specified for the feeds and products of each unit process. Each SNM/bulk determination method can specify a measurement or combination of measurements to determine total SNM or SNM concentration, and a measurement or combination of measurements to determine material bulk. The specific measuring instruments that may be used for each measurement can be specified. One of the SNM determination methods that may be specified is "weight times factor." When the final SNM measurement result for a determination method will be delayed, the method can specify a measurement or combination of measurements to determine a provisional SNM value.

Feed/product measurement specifications. One or more SNM/bulk determination methods can be specified for each feed and product category for every unit process. When a (by-)product must be accumulated over several operating cycles of a unit process to generate a batch, SNM/bulk determination methods may be specified for the increment from each cycle, for the batch, for both, or for neither. If more than one SNM/bulk determination method is given for a material, these are tried in order until a method is found for which at least one of the required measuring instruments is available.

The addition of this set of elements to the simulation model has proved to be adequate to provide a flexible and detailed description of SNM measurement and accounting procedures in an SNM processing facility. In the next section we shall illustrate this by describing simulations that were performed for a fictitious nuclear material processing line.

4. Application to an Example Process Line

In Ref. 1 we described the application of our simulation model to two versions of a fictitious pyrochemical process line for converting plutonium oxide to pure plutonium metal. We shall use the simpler of these process-line versions here to illustrate the simulation of material measurement and accounting procedures. The example pyrochemical process line is shown schematically in Fig. 1. Plutonium oxide from the vault is converted

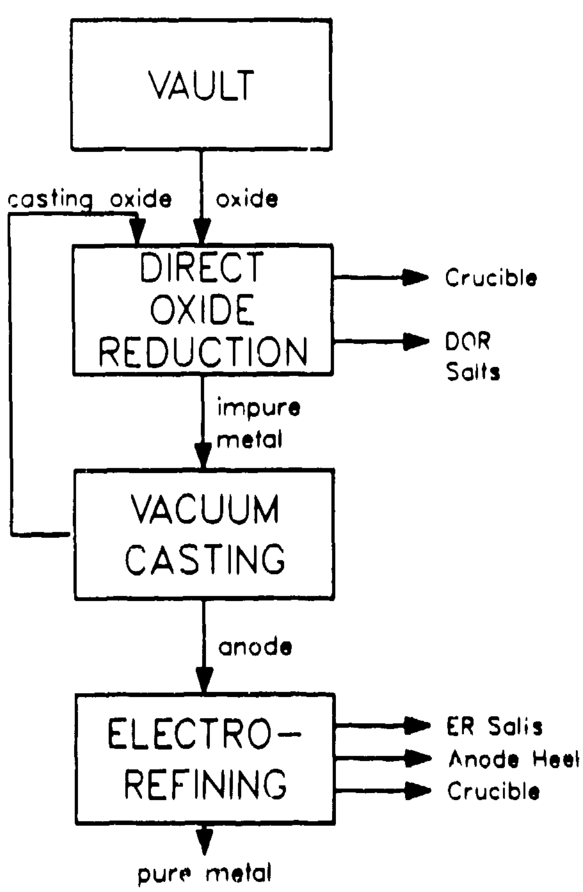

Fig. 1.
Schematic representation of a fictitious pyrochemical processing line for converting plutonium oxide to pure plutonium metal.

Table 1. Feeds and products of the unit processes in the fictitious plutonium processing line.

Process	Units	Feed	Products	Destination
DOR	5	Oxide	Impure metal	CASTING*
			DOR salts	Waste
			Crucibles	Waste
CASTING	1	Imp metal	Anode	ER*
			Oxide	DOR*
ER	1	Anode	Pure metal	Vault
			Anode heel	Vault
			ER salts	Vault
			Crucibles	Waste

*Or the vault

to impure plutonium metal in one of five direct oxide reduction units (DOR). This impure metal is sent to a vacuum casting unit (CASTING), where a batch of the impure metal is accumulated and cast into an anode. The anode is sent to the electrorefining unit (ER), where it is converted to pure metal. Impure metal that cannot be accepted by CASTING and anodes that cannot be accepted by ER are sent to the vault. CASTING produces plutonium oxide as a by-product, and this oxide is recycled to DOR. In addition, DOR and ER produce byproducts that are sent to the vault or to waste storage. The feeds and products of each of the unit processes are shown in Table 1. Assumed batch sizes and processing time requirements for the unit processes are given in Ref. 1.

The measuring instrument types used in the simulation, the number of instruments assumed for each type, and the calibration frequency for each instrument are shown in Table 2. The material accuracies used for the gamma spectrometer are given in Table 3, as an example of the types of information that may be specified. All calibration and precision uncertainties were assumed to be purely multiplicative except those for the balances, which were assumed to be purely additive.

Table 2. The instrument types, numbers of instruments, and calibration schedules used in the simulation.

Instrument Type	Number	Calibration Schedule
Balance	2	Weekly
Calorimeter	2	Monthly
Chemistry	2	Weekly
Gamma spectrometer	1	Monthly
Neutron counter	1	Bimonthly

Table 3. The material accuracies assumed for the gamma spectrometer. All uncertainty distributions were assumed to be normal with zero mean, and additive precision and calibration errors were taken as zero.

Materials	Multiplicative Calibration Error Std Deviation	Multiplicative Precision Error Std Deviation
ER salts, DOR salts	0.05	0.02
Oxide, anode, anode heel	0.005	0.01
Crucible	0.15	0.1

The source of feed material for the process line was an initial inventory of plutonium oxide in the vault. The oxide items withdrawn from the vault were given errors in their mass and SNM values typical of measurement by weighing and chemical analysis. Because all items entering processes had reasonably good measured values from previous process steps or the vault, no feed measurements were made. The SNM determination methods used for the products of the unit processes are shown in Table 4.

Because of the small size of the process line, only three MBAs were initially used in the simulation: one for the vault, one for waste storage, and one for the entire process line containing the DOR, CASTING, and ER units. Each MBA area had a monthly balance closure, performed late in the day on the last day of the month. Because only the process MBA contains material measurement points, it is the only one of the three MBAs that can have a nonzero ID arising from measurement uncertainties.

Operation of the fictitious facility was simulated for a seven-month period from 12/1/86 to 6/30/87. The simulation was begun with no feed for CASTING or ER, so the first month of simulated time was used to establish a (relatively) steady process state; and only the material balance closures for the last six months of the period were used in evaluating IDs. The beginning and ending inventories and the SNM additions and removals found for the process MBA for each of these six balance periods are shown in Table 5.

The sample variance for these six IDs is 69 860 g^2 Pu, corresponding to an estimated standard deviation of 278 g Pu for the ID (assuming the IDs are normally distributed). This standard deviation is a small fraction of monthly

Table 4. SNM/bulk determinations for the products of the unit processes. Only the SNM measurements are shown; each determination also uses a mass measurement on one of the two balances. Increment measurements are those made for the output of a single process cycle when several process cycles are required to form a batch.

Unit Process Material	Increment SNM Measurement	Batch SNM Measurement
DOR		
Impure metal	None	Weight times factor
DOR salts	None	Neutron count/ gamma spec
Crucible	None	Neutron count/ gamma spec
CASTING		
Anode	None	Calorimetry/ gamma spec
Oxide	Weight times factor	Calorimetry/ gamma spec
ER		
Pure metal	None	Chemistry
Anode heel	None	Calorimetry/ gamma spec
ER salts	None	Calorimetry/ gamma spec
Crucible	None	Neutron count/ gamma spec

Table 5. Material balance closure figures for the process MBA of the fictitious pyrochemical process line for six monthly balance periods in the interval 1/1/87 through 6/30/87. Because of rounding, some of the IDs differ by one unit from the values calculated from the inventory information shown.

Period	Initial Inventory (g Pu)	Additions (g Pu)	Final Inventory (g Pu)	Removals (g Pu)	ID (g Pu)
1	12 344	122 147	21 033	113 254	-204
2	21 033	107 673	18 442	109 975	-289
3	18 442	114 322	17 739	115 229	204
4	17 739	105 576	19 630	103 811	126
5	19 630	100 163	20 682	99 125	15
6	20 682	113 835	15 965	118 975	423

material throughput for the process MBA, a result of the fact that the measurements for all the feed entering the MBA and most of the products leaving the MBA are high-accuracy measurements (chemistry) on good-quality material (oxide and pure metal).

We shall give one other illustration of the use of the measurement simulation model by examining another configuration of process MBAs for our fictitious facility. Let us suppose that spatial contiguity considerations at the facility dictate that the DOR units be placed in one MBA and the CASTING and ER units in another. It requires less than a minute's time to alter the facility data files for the previous case to reflect this revised MBA structure, and after the same seven-month simulation has been run one obtains the balance closure information shown in Table 6. The estimated variance of the MBA containing DOR, based on the six results shown, is 7342 g^2, and the estimated variance for the MBA containing CASTING and ER is 49 784 g^2. However, an interesting new feature has appeared: it is apparent that there are biases in the ID values for the two MBAs. Reference to Table 4 shows that the SNM in the impure metal transferred from DOR to CASTING is determined on a weight-times-factor basis, and the factor used is clearly not quite large enough. The error in the factor used by DOR did not make itself evident for the previous choice of MBAs because there it did not appear in measured values of items crossing MBA boundaries. To eliminate the bias one could now adjust the value upward slightly, run additional simulations and check the new IDs, and continue this adjustment process until the bias becomes negligible. An alternative approach would be to evaluate new SNM determination methods for the impure-metal product of DOR that are not so prone to bias.

5. Discussion

In the preceding section of this paper we have described two simple applications of the material measurement and accounting features of the enhanced simulation model. The information about IDs from these simulations that we have presented here is only a minuscule part of the measurement information that was actually generated during the simulations, and in fact the estimates of variances for MBA IDs (though not the biases) could have been obtained easily in this case by a propagation-of-errors approach. However, if we had wished to do so, we could have accessed additional detailed simulation information about thousands of individual measurements performed during the course of the simulations, including when and where each measurement was performed, by whom, and what the measurement error was. In addition, we could have examined every transfer of materials between MBAs to determine the time of transfer, the materials transferred, and the operators involved in the transfer. Additional information could have been obtained about measuring instrument usage and measurement bottlenecks, the times delayed-measurement results were received and applied to update MBA records, etc. This abundance of detailed measurement and accounting information provided by simulation permits one to make a more comprehensive study of the expected operating characteristics of the material accounting system by this method than by any other approach except extensive observation and experimentation in the facility itself.

Table 6. Material balance closure figures for the case of two process MBAs for six monthly balance periods in the interval 1/1/87 through 6/30/87. Because of rounding, some of the IDs differ by one unit from the values calculated from the inventory information shown.

Period	Initial Inventory (g Pu)	Additions (g Pu)	Final Inventory (g Pu)	Removals (g Pu)	ID (g Pu)
		MBA containing DOR			
1	4 037	94 086	4 092	93 590	-442
2	4 092	81 932	4 125	81 658	-240
3	4 125	85 961	4 000	85 616	-469
4	4 000	94 305	4 046	93 923	-337
5	4 046	86 078	4 043	85 752	-329
6	4 043	90 097	4 099	89 729	-312
		MBA containing CASTING and ER			
1	8 156	97 535	16 955	88 705	- 31
2	16 955	85 937	14 136	88 569	-187
3	14 136	81 280	13 563	82 206	354
4	13 563	79 803	15 387	78 154	176
5	15 387	76 280	15 687	76 187	207
6	15 687	84 977	11 660	89 394	390

Reference

1. C. A. Coulter, K. E. Thomas, C. L. Sohn, T. F. Yarbro, and K. W. Hench, "A Facility Model for the Los Alamos Plutonium Facility," Nucl. Mater. Manage. XV, 171 (1986).